

4-Phenyltoluene
644-08-6 | DTXSID4047177

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 280 °C

Global applicability domain: Inside

Local applicability domain index: 7.16e-01

Confidence level: 7.91e-01

Nearest Neighbors from the Training Set

Image not found

Naphthalene, 1-(chloromethyl)-

Measured: 292

Predicted: 270

Image not found

Acenaphthene

Measured: 279

Predicted: 270

Image not found

Naphthalene, 1-allyl-

Measured: 266

Predicted: 272

Image not found

1,6,7-Trimethylnaphthalene

Measured: 285

Predicted: 269